MODELING OF CO_2 SOLUBILITY IN METHYLDIETHANOLAMINE + PIPERAZINE AQUEOUS SOLUTIONS USING NEURAL NETWORK MODEL

by

AHMAD NAJDAN BIN NASERI

Dissertation submitted in partial fulfilment of

the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

SEPTEMBER 2012

Universiti Teknologi PETRONAS

Bandar Seri Iskandar

31750 Tronoh

Perak Darul Ridzuan

CERTIFICATION OF APPROVAL

MODELING OF CO_2 SOLUBILITY IN METHYLDIETHANOLAMINE + PIPERAZINE AQUEOUS SOLUTIONS USING NEURAL NETWORK MODEL

by

AHMAD NAJDAN BIN NASERI

A project dissertation submitted to the
Chemical Engineering Programme
Universiti Teknologi PETRONAS
in partial fulfillment of the requirement for the
BACHELOR OF ENGINEERING (Hons)
(CHEMICAL ENGINEERING)

Approved by,

_____

(Ir. Dr. Abd Halim Shah Bin Maulud)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
Sept 2012

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

_____

AHMAD NAJDAN BIN NASERI

ABSTRACT

Acid gas removal processing from natural gas, synthesis gas and refinery gas stream is very important in plant industry to prevent corrosion in the subsequent piping and as per required by users. Generally, the gaseous feedstock stream is contacted with alkanolamine aqueous solution countercurrently in the acid gas absorber tower. The acid gas will partly be converted to non-volatile ionic species by the basic amine and partly be dissolved physically in the liquid solution. Acid gas removal unit is very important in petrochemical processing plant.

There had been great numbers of studies on the solubility of CO_2 in methyldiethanolamine (MDEA) aqueous solutions. M. Vahidi used extended Debye-Huckle model to explain on the solubility data of CO_2 absorption in MDEA and Piperazine (PZ) at certain concentration, temperature and pressure. The average absolute relative deviation percent (AAD %) reported were 8.11%.

Model of solubility of CO2 in MDEA aqueous solution using neural network model is presented. In this work, neural network was used to determine solubility of CO2 in MDEA + PZ solutions based on 3 experimental research data, M. Vahidi (Mehdi Vahidi, 2009), H. B. Liu (Hua-Bing Liu, 1999) and B. Si Ali (B. Si. Ali, 2004). Data prediction was conducted at different temperature and partial pressure and for various solution concentrations. The model developed has an absolute relative deviation of 3.047% compared to other papers; M. Vahidi with 8.11% deviation, B. Lemoine of 7.84% and H. B. Liu with 11.6% error deviation. The model also not capable to extrapolate prediction of CO_2 loading on zero promoter system due to the experimental data at zero promoter is not included in the training process.

ACKNOWLEDGEMENTS

First and foremost, I would like to express my praises to God for His blessing in completing this thesis. Special appreciation and sincere gratitude is extended to my supervisor, Ir. Dr. Abd Halim Shah Bin Maulud for patience, motivation, enthusiasm, and immense knowledge throughout the Final Year Project II to fulfill the university requirement. His invaluable guidance helped me in all the time of research and writing of this thesis.

My sincere thanks also goes to Final Year Project (FYP) coordinator, Dr. Nurhayati Mellon for their encouragement and stringent in handling the course effectively throughout the year. The management of the FYP is systematic and every submission datelines are perfectly scheduled.

Special thanks to all my fellow coursemates also other lecturers who have always been accommodating and cooperative for their kindness in giving of ideas, opinion and moral support throughout the completion of this project report.

Last but not least, I would like to acknowledge my family members for supporting me motivated and spiritually throughout the year.

Thank you.

LIST OF FIGURES

LIST OF TABLES

TABLE OF CONTENTS

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

Acid gas absorption process is widely used in petrochemical processing industry. Generally, the gaseous feedstock stream is contacted with alkanolamine aqueous solution countercurrently in the acid gas absorber tower to absorb the acid gas (CO_2 and H_2S). The absorbent or alkanolamine is normally washed by steam stripping in the water stripper section for recovery. The acid gas will partly be converted to non-volatile ionic species by the basic amine and partly be dissolved physically in the liquid solution. Acid gas removal unit is very important in petrochemical processing plant. It can cause cause corrosion to the pipeline because it can react with moisture to form a carbonic acid. Nowadays, among the most effective and economic acid gas removal is by using package blended amine, in this case MDEA in aqueous solution. This research focused on the percentage removal efficiency of CO_2 based on parameters such as MDEA aqueous solution concentration in an absorption unit.

There have been great numbers of investigations on the solubility of CO_2 in MDEA aqueous solutions. M. A. Pacheco et al. (Manuel A. Pacheco, 2000) and Q. Zhi and G. Kai (Kai, 2009) studied the effect of the reaction kinetics and thermodynamic parameters interaction on the interfacial mass transfer rates of CO_2. Both parties have developed a mathematical model to interpret and analyze the experimental data. Their modeling aid a lot in chemical technologies growth to create a more effective sour gas absorbent.

Many studies also have been performed on the kinetics of reaction of CO_2 with MDEA aqueous solution. Jiun-Jie Ko et al. (Jiun-Jie Ko, 2000) and Chin-Yuan Lin et al. (Chih-Yuan Lin, 2009) studied on the physical properties such as solubility and diffusivity of acid gases in amine solutions. This information is very important for rational design of the gas absorption unit. Both paper directly applied Versteeg and van

Swaaij (Versteeg, 1988a) in their study to calculate the corresponding solubility and diffusivity of CO_2 in amine solution.

M. Vahidi et al. (Mehdi Vahidi, 2009) used extended Debye-Huckle model to explain on the solubility data of CO_2 absorption in MDEA of concentration (2.52, 3.36, and 4.28) kmol/m^3, at temperature (313, 323 and 343) K and partial pressures ranging from about (30 to 5000) kPa. The effects of piperazine (PZ) concentration on CO2 loading in MDEA aqueous solutions were determined at PZ concentration (0.36, 0.86 and 1.36) kmol/m^3. In this work, neural network model will be developed to predict the solubility of CO2 in MDEA-CO2-H2O system at various operating parameter and concentrations. The developed model later on will be used to predict MDEA system with and without the promoter and compare the performance of the established model with the experimental data based on error analysis.

1.2 PROBLEM STATEMENT

M. Vahidi et al has conducted an experiment at various temperatures, pressure and aqueous MDEA and PZ concentration, where the interaction parameters of activity coefficient model of these systems are determined. The results shows the beneficial mixture of piperazine (PZ) + MDEA to the CO_2 loading is better. The average absolute relative deviation percent (d_{AAD}) for all data points were 8.11% (Mehdi Vahidi, 2009).

On the same experimental data from above paper by M. Vahidi et al. (Mehdi Vahidi, 2009), H. B. Liu et al. (Hua-Bing Liu, 1999) and B. S. Ali et al (B. Si. Ali, 2004), the prediction with respect to artificial neural network model will be developed. The motivation of the studied system is basically to test the performance of neural network model respond to MDEA-CO2-H2O system with presence and absence of Piperazine in the system.

1.3 OBJECTIVE

1. To develop a neural network model for MDEA-CO2-H2O system based on experimental data of M. Vahidi et al. (Mehdi Vahidi, 2009), H. B. Liu et al. (Hua-Bing Liu, 1999) and B. S. Ali et al (B. Si. Ali, 2004), the research paper studied on sour gas absorption in MDEA + PZ solution.
2. To predict the model at different operating condition and to analyze on the performance at different experimental data.

1.4 SCOPE OF STUDY

This research paper mainly focuses on the solubility of CO_2 in MDEA + PZ solution. It will partly cover on neural network model to study on the absorption of acid gaseous. B. Lemoine et al. (B. Lemoine, 2000) had studied on the solubility of CO_2 and H_2S in aqueous solution MDEA. They used the simplified Clegg-Pitzer equation for the modeling of the studied system. Back to the objective of this paper, the deviation is then will be compared with experimental data of MDEA-CO2-H2O system.

CHAPTER 2

LITERATURE REVIEW

2.1 ACID GAS

Acid gas is natural gas or any other gas mixture which contains significant amounts of hydrogen sulfide (H_2S), carbon dioxide (CO_2), or similar contaminants. The terms acid gas and sour gas are often incorrectly treated as synonyms. For instance, a sour gas is any gas that specifically contains H_2S in significant amounts whereas an acid gas is any gas that contains significant amounts of acidic gases such as CO_2 or H_2S. Thus, CO_2 by itself is an acid gas but not a sour gas (Citizendium). This project mainly focus on CO_2 removal where will be discussed more afterwards.

CO_2 composed of two oxygen atoms covalently bonded to a single carbon atom. It is a gas at Standard temperature and pressure. It exists as a trace gas at a concentration of 0.039% by volume in ambient. This gas involve in carbon cycle process which is known as photosynthesis. Plants, algae, and cyanobacteria absorb carbon dioxide, light, and water to produce carbohydrate energy for themselves and oxygen as a waste product. Carbon dioxide is also produced by combustion of coal or hydrocarbons, the fermentation of liquids and the breathing of humans and animals (Shakhashiri, 2008).

As we all know CO_2 is colorless, at low concentrations the gas is odorless and at higher concentrations it has a sharp, acidic odor. At standard temperature and pressure, the density of carbon dioxide is around 1.98 kg/m^3, about 1.5 times that of air. At 1 atmosphere, the gas deposits directly to a solid at temperatures below −78.5 °C and the solid sublimes directly to a gas above −78.5 °C. In its solid state, carbon dioxide is commonly called dry ice. Phase diagram of CO_2 is as shown in Figure 2.1.

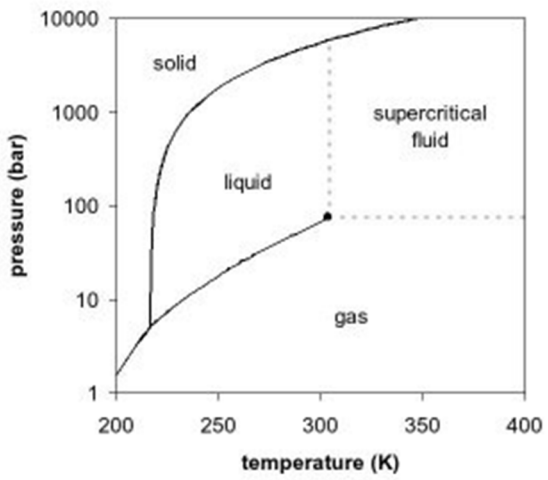


Figure 2.1 : Carbon dioxide pressure-temperature phase diagram

The carbon dioxide (CO_2) can cause global warming. Carbon dioxide doesn't absorb the energy from the sun, but it does absorb some of the heat energy released from the earth. When a molecule of carbon dioxide absorbs heat energy, it goes into an excited unstable state. It can become stable again by releasing the energy it absorbed. Some of the released energy will go back to the earth and some will go out into space. So in effect, carbon dioxide lets the light energy in, but doesn't let all of the heat energy out, similar to a greenhouse (MSU Science Theatre, 1994). Furthermore, in natural gas, if more than 3% of CO_2 composition contains, the gas is unmarketable. CO_2 can also cause corrosion to the pipeline. Nowadays, among the most effective and economic acid gas removal is by using amine unit, in this case MDEA in aqueous solution. This research focused on the solubility of CO_2 modeling in MDEA aqueous solution concentration in an absorption unit. MSDS regarding CO2 are provided in Appendix 1.

2.2 ALKANOLAMINES

The removal of acid gas such as carbon dioxide (CO_2) is very important in industrial process. There are some numbers of inventions on this system, but the most commonly used method is amine system absorption unit such as by using diethanolamine (DEA), methyldiethanilamine (MDEA), etc. The method couples the physical absorption together with chemical reaction which partially changes the chemical in the solution into carbonates, bicarbonates and carbamates depend on the type of amine used (M. Z. Haji-Sulaiman, 1996).

In this work, MDEA will be used as CO_2 carrier. Methyldiethanolamine (MDEA) solutions nowadays have found an increased used with advantages of H2S selective removal and lower enthalpy of reaction and vapor pressure compare to primary and secondary alkanolamines aqueous solutions. Shown below in Figure 2.2 is the molecular structure of MDEA. MSDS on MDEA is provided in Appendix 2.

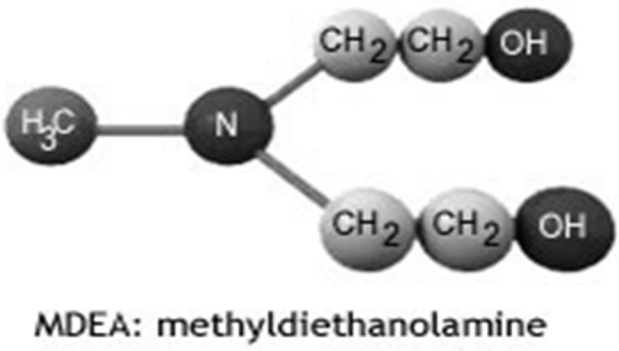


Figure 2.2: Molecular structure of methyldiethanolamine (MDEA)

Versteeg and Van Swaaij have studied that the absorption of CO_2 into MDEA aqueous solution could be described completely as a physical absorption. It was almost identical to the absorption of N2O, corrected for the differences in physical constants, in the same solution. Moreover, the total amount of CO_2 absorbed was nearly the same as the amount which can be physically dissolved in this solution. They were able to ascribe the differences completely to the presence of primary and secondary amine impurities (Versteeg, 1988a).

2.3 ABSORPTION PROMOTER

Due to low reaction rate of the CO_2 absorption by alkanolamines, promoters or activators are needed to improve the removal process. The following compounds can be used to increase the reaction rate:

- Formaldehyde
- Methanol
- Phenol
- Ethanolamine
- Arsenious acid
- Glycine
- Hinderd amine

The general mechanism for promoted solutions is as below:

$$CO_2 + \text{promoter} \leftrightharpoons \text{intermediate}$$

$$\text{intermediate} + OH^- \leftrightharpoons \text{promoter} + HCO_3^-$$

The addition of a primary or secondary amine to a tertiary amine has found wide-spread application in the absorption and removal of CO_2 from process gases. PZ is most active as promoter when used in combination with MDEA, therefore the most attention is focused to articles concerning this combination (Lensen, 2004).

In table 2.1 shows an overview of the chemical data of PZ.

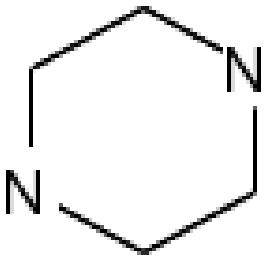
Synonyms:	**Piperazine Anhydrous, Diethylenediamine**
Molecular Formula:	$C_4H_{10}N_2$
Formula Weight:	86.13
Registry number:	110-85-0
Density:	146
Melting point:	108-112^{o}C
Boiling Point:	145-146^{o}C
Flash point:	82^{o}C
Structure:	

Table 2.1: Chemical data of piperazine

PZ may be synthesized by, for example, reacting monoethanolamine with ammonia, or reacting ethylene oxide and NH_3 and cyclizing the ethanolamines thereby obtained (M. Appl, 1980). The ability of a solvent to remove carbon dioxide is dictated by its equilibrium solubility as well as mass transfer and chemical kinetics characteristics.

2.4 NEURAL NETWORK

Neural Networks is a classification of Artificial Intelligence (AI) where we, by motivation from the human brain, find set of data structures and algorithms for education and organization of data. Many tasks that humans perform naturally firm, such as the recognition of a familiar face, proves to be a very complicated task for a computer when conventional programming methods are used. By applying Neural Network techniques a program can learn by examples, and create an internal structure of rules to classify different inputs, such as recognizing images.

The Neuron

The simple neuron model is made from studies of the human brain neurons. A neuron in the brain receives its chemical input from other neurons through its dendrites. If the input exceeds a certain threshold, the neuron fires its own impulse on to the neurons it is connected to by its axon. Below is a very simplified figure as each of the neurons of the brain is connected to about 10000 other neurons. (Nielsen, 2001)

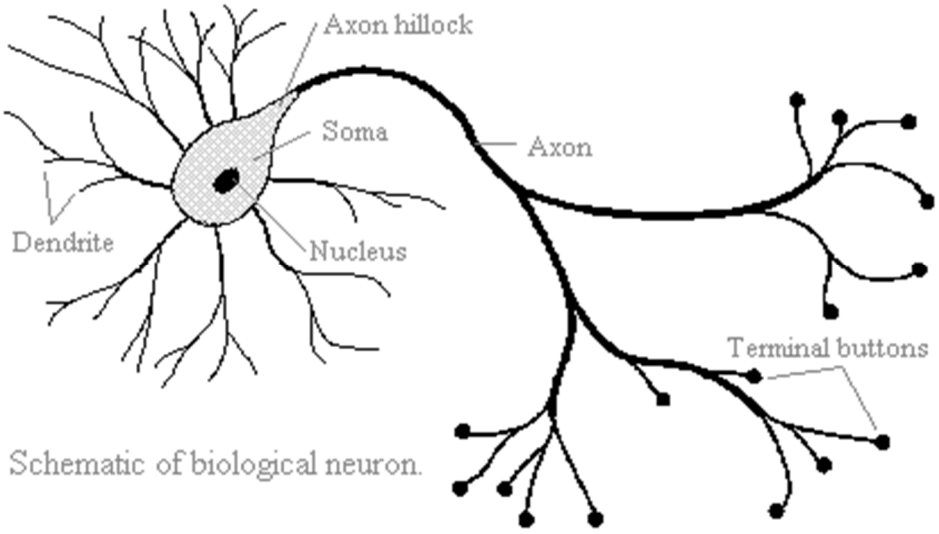


Figure 2.41 : Illustration of neuron model

The Perceptron

The simple perceptron models this behavior in the following way. First the perceptron receives several input values (x0 - xn). The connection for each of the inputs has a weight (w0 - wn) in the range 0-1. The Threshold Unit then sums the inputs, and if the sum exceeds the threshold value, a signal is sent to output. Otherwise no signal is sent.

The perceptron can learn by adjusting the weights to approach the desired output. With one perceptron, it is only possible to distinguish between two pattern classes, with the visual representation of a straight separation line in pattern space (Illustration 8 Pattern Space).

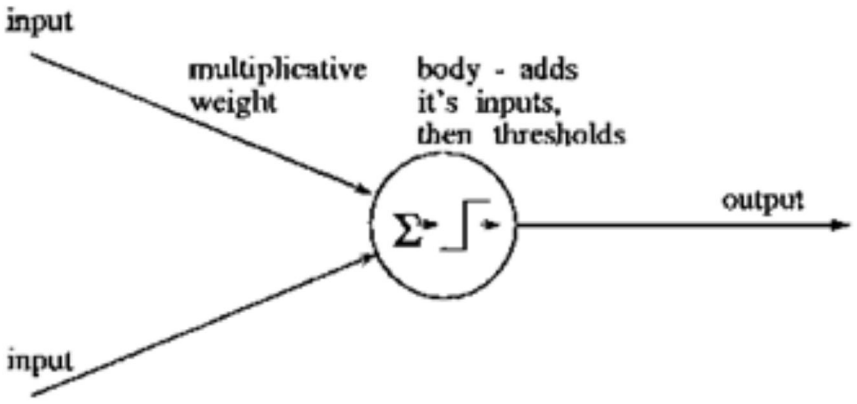


Figure 2.42 : Illustration of perceptron model

The multilayer Perceptron (MLP) network

Building on the algorithm of the simple Perceptron, the MLP model not only gives a perceptron structure for representing more than two classes, it also defines a learning rule for this kind of network.

The MLP is divided into three layers: the input layer, the hidden layer and the output layer, where each layer in this order gives the input to the next. The extra layers give the structure needed to recognize non-linearly separable classes.

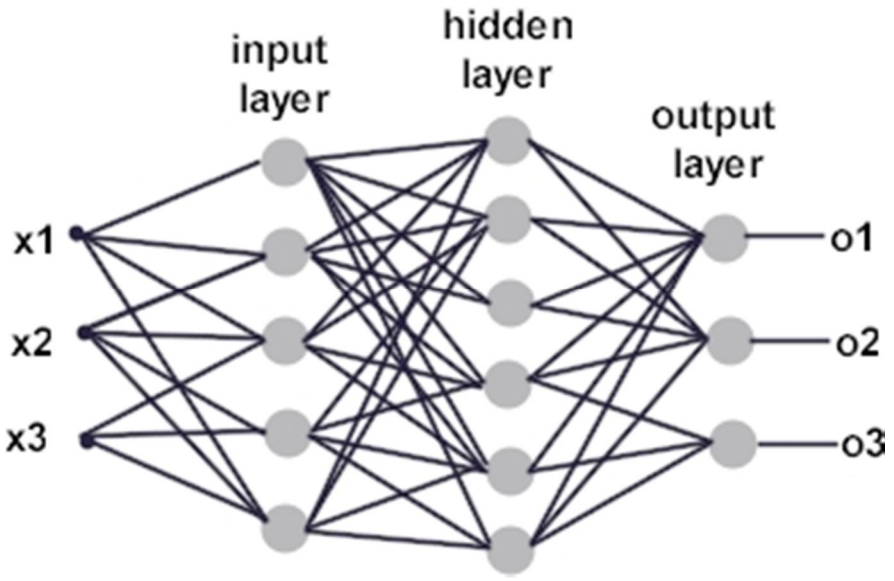


Figure 2.42 : The Multi Layer Perceptron

Algorithm

The threshold function of the units is modified to be a function that is continuous derivative, the Sigmoid function (Formula 4 The Sigmoid Function). The use of the Sigmoid function gives the extra information necessary for the network to implement the back-propagation training algorithm. Back-propagation works by finding the squared error (*the Error function*) of the entire network, and then calculating the error term for each of the output and hidden units by using the output from the previous neuron layer. The weights of the entire network are then adjusted with dependence on the error term and the given learning rate. (Formula 6 MLP Adapt weights)

Training continues on the training set until the error function reaches a certain minimum. If the minimum is set too high, the network might not be able to correctly classify a pattern. But if the minimum is set too low, the network will have difficulties in classifying uneven patterns.

Applications for Neural Networks

Neural Networks are successfully being used in many areas often in connection with the use of other AI techniques. A classic application for NN is image recognition. A network that can classify different standard images can be used in several areas:

- ✓ Quality assurance, by classifying a metal welding as whether is holds the quality standard.
- ✓ Medical diagnostics, by classifying x-ray pictures for tumor diagnosis.
- ✓ Detective tools, by classifying fingerprints to a database of suspects.

A well known application using image recognition is the Optical Character Recognition (OCR) tools that we find available with the standard scanning software for the home computer. Scansoft has had great success in combining NN with a rule based system for correctly recognising both characters and words, to get a high level of accuracy1.

All the network topologies and algorithms have their advantages and disadvantages. When it comes to understanding the spoken language the best found solutions use a combination of NN for phoneme recognition and an Expert system for Natural language processing, where neither AI technique can be adapted to solve the problem in whole. Kohonen himself succeeded in creating a 'phonetic typewriter' by using his self-organising networks for the phoneme recognition and a rule base for applying the correct grammar.

Another popular application for NN is Customer Relationship Management(CRM).
Many companies have at the same rate as electronic data storage has become commonplace built up large customer databases. By using Neural Networks for data mining in these databases, patterns however complex can be identified for the different types of customers, thus giving valuable customer information to the company.

One example is the airline reservation system AMT2 which could predict sales of tickets in relation to destination, time of year and ticket price. The NN strategy was well

suited for the purpose because the system could be updated continuously with the actual sales.

In relation to the recent trends in Management strategies CRM has reached a high priority, because of the prospects of a successful CRM system adding value to the business in terms of not only better prediction of customer needs but also predicting which customers will be the most valuable for the company.

Some rules of thumb exist for evaluating whether a problem is suitable for a Neural Network implementation:

- ✓ There must be a large example dataset of the problem in order to be able to train the network.
- ✓ The data relationships in the problem are complex and difficult or impossible to program using conventional techniques.
- ✓ The output does not need to be exact or numeric.
- ✓ The desired output from the system changes over time, so a high flexibility is needed.

CHAPTER 3

METHODOLOGY

3.1 PROJECT METHODOLOGY

Figure 3.1 explain on the methodology steps of the project.

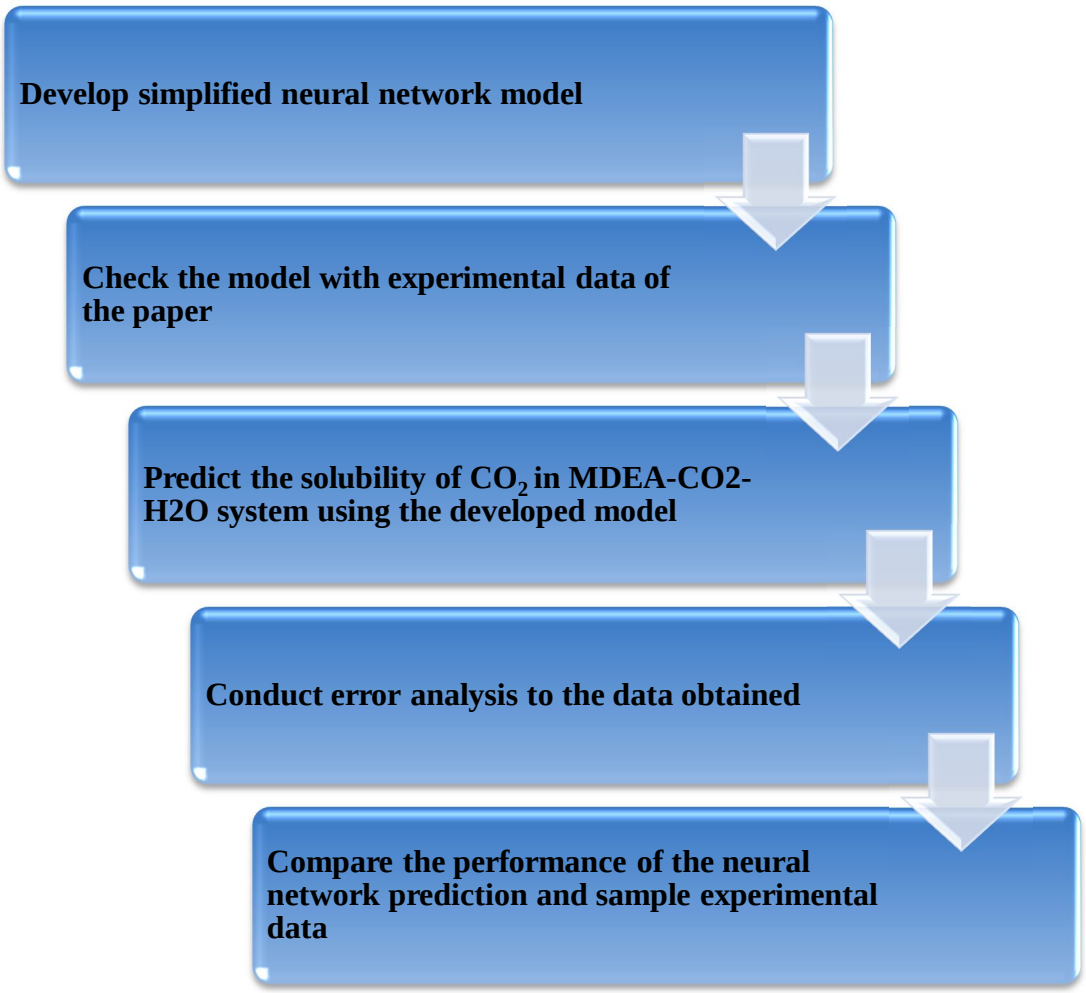


Figure 3.1: Project Flowchart

The systematic study of methods regarding this project covers 5 basic important steps which as shown above. For initiation of this study case, development of neural network model comes first. The model will be generated by using MATLAB software which is high-technical algorithm development software. The models covered are to determine the optimum number of neuron and also analysis of error to compare the performance of the models.

After that, the model will be tested with experimental data from M. Vahidi et al. (Mehdi Vahidi, 2009), H. B. Liu et al. (Hua-Bing Liu, 1999) and B. S. Ali et al (B. Si. Ali, 2004) research paper. This process is to ensure that the neural network model developed is valid. Mean square error and regression of the results will be calculated for each run and the the optimal neuron number is determined based on MSE and R obtained. (MSE = 0 = accurate; R = 1 = precise) Then it will be used to predict the solubility of CO_2 at different operating condition and also test on MDEA-CO2-H2O system without promoter when PZ = 0.

Next, error analysis to the result data will be conducted to check the accuracy of this model, how it respond to system without introducing promoter. The analysis conducted will be based on the comparison of the experimental value and predicted value from the model. Finally, the results will be presented in graph form for further analysis and understanding.

3.2 GANTT CHART

Table 3.1 shows the Gantt Chart for proposal development.

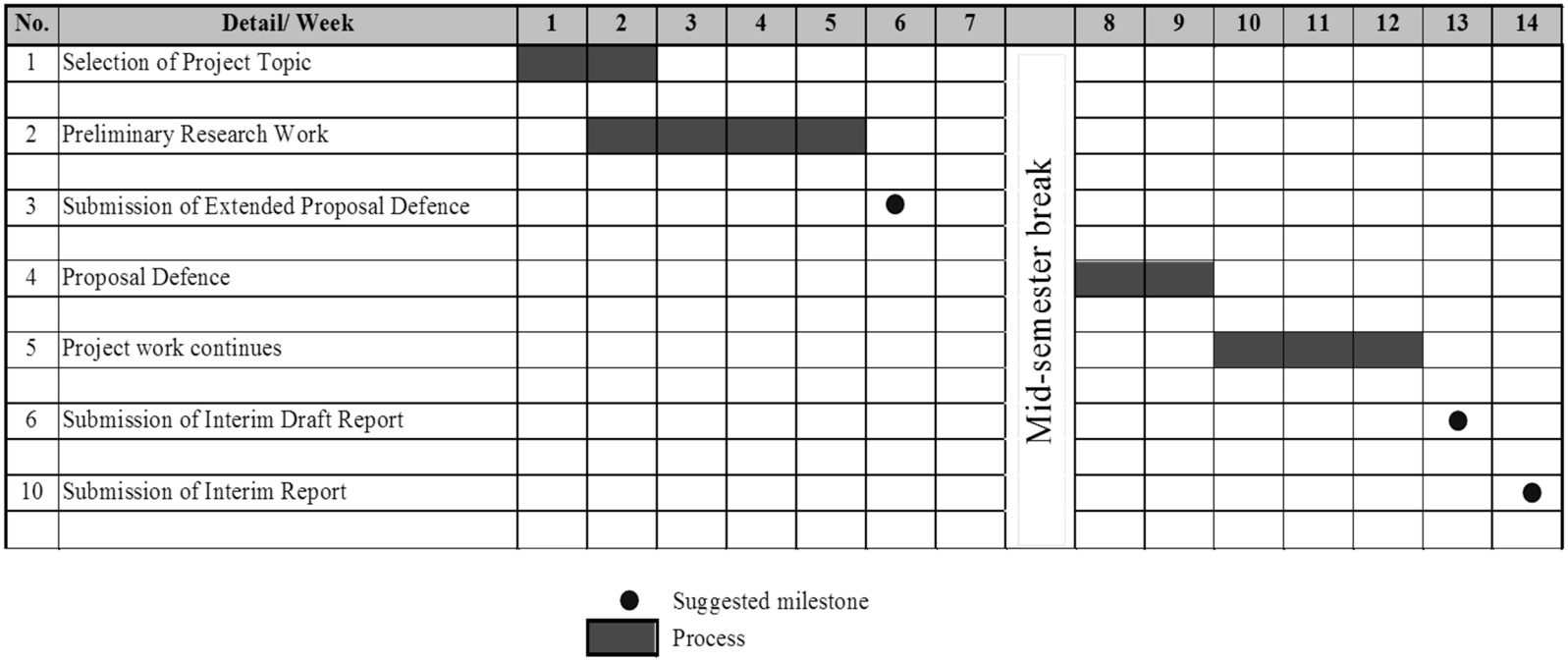


Table 3.1: Proposal Gantt Chart

Gantt chart is primarily a method by which time management for any activity is undertaken. It shows up a break up of how time is utilized when performing different set of activities while working on any project. It has a simple gapping representation of a project with start and end dates for each phases. Gantt chart is useful in the fact that it is understandable by a large number of audiences. It has many applications in all fields.

From table above, basically there are 7 main item targeted to finish by this semester. From the table, 3 elements were targeted to complete before mid-semester break and planning others to completion afterwards. Further details regarding the project planning are as shown in table above.

3.3 SOFTWARE REQUIRED

Throughout this project, the main software needed to run this model are:

a) Microsoft Excel
b) MATLAB

CHAPTER 4

RESULT AND DISCUSSION

To ensure the reliability of the experimental data, it is important that the data is taken at random for each run and the amount of training data should be kept constant. In development of this model, data for training is set to 60%, 5% for validation and 35% for testing. Analysis on the mean square error and regression was performed at end of each run. Targeted MSE is 0 (most accurate) and R is 1 (most precise). For every run, the measured MSE and R were monitored and included in error analysis. Thus, the best number of neuron can be determined. Table below shows the number of neuron set in each run with MSE and R obtained.

Neuron	Epoch	MSE (Training)	R (Training)	MSE (Test)	R (Test)
1	50	1.43E-02	9.23E-01	1.73E-02	9.22E-01
2	115	3.04E-03	9.86E-01	3.53E-03	9.83E-01
3	37	1.35E-03	9.94E-01	2.43E-03	9.88E-01
5	46	1.26E-03	9.94E-01	2.63E-03	9.87E-01
7	25	1.07E-03	9.95E-01	2.60E-03	9.86E-01
10	60	6.53E-04	9.97E-01	1.96E-03	9.89E-01
11	55	2.47E-03	9.95E-01	2.03E-03	9.81E-01
12	43	3.07E-03	9.83E-01	7.39E-03	9.66E-01
15	29	5.88E-03	9.74E-01	9.00E-03	9.55E-01
20	8	2.09E-02	9.17E-01	2.19E-02	9.16E-01
30	15	1.27E-02	9.43E-01	2.26E-02	8.85E-01

Table 4.1 : Results

From table above, the least MSE and R can be obtained when number of neuron is set to 10 where mean square error = 6.53e-4 and regression = 9.97e-1. Further analysis of the result is as illustrated in graph below.

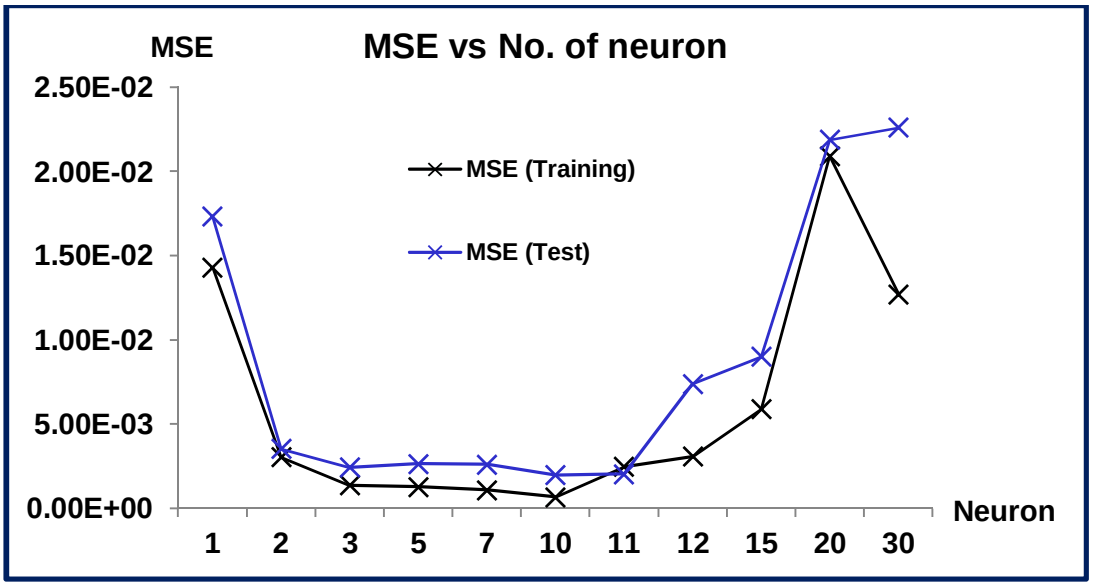


Figure 4.1 : Graph of MSE vs No. of neuron

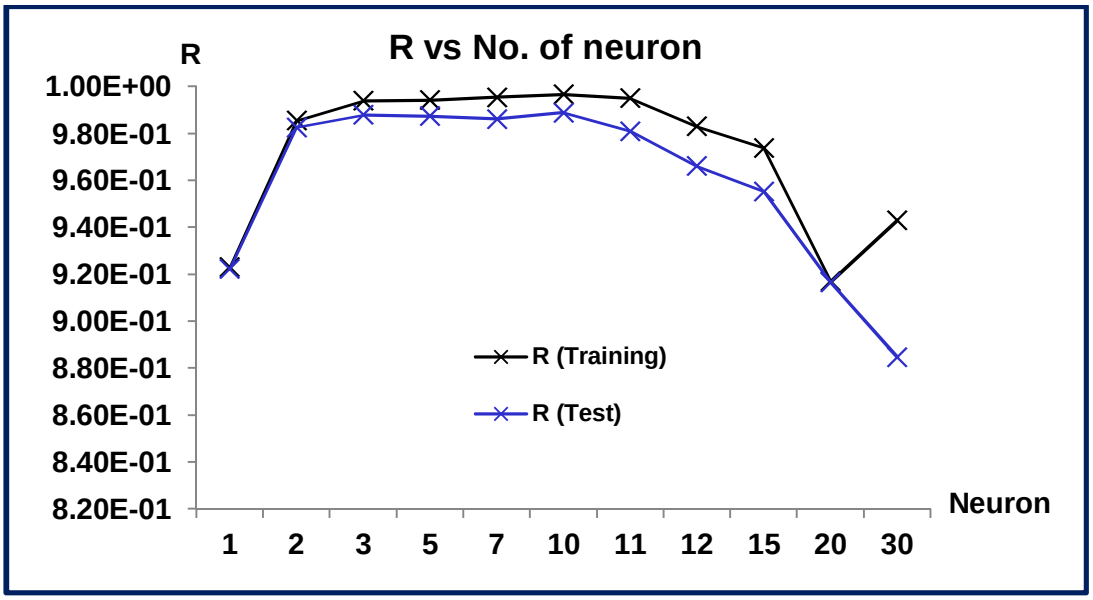


Figure 4.2 : Graph of R vs No. of neuron

Hence, for this neural network model, extremum neuron can be obtained at 10, which the model would give the minimum MSE and maximum value of R. The epoch obtained at this neuron number is at 60; when the network built has provide an optimal generalization performance. The general form of this model can be classified as early-stopping interpretation, this effectively explain that the network is not over-fit its training data and

generalized well. Over-fitting occurs when epoch number reaches 1000 which the models or equations generated for the data is too many and cannot be generalized.

The deviations of the model toward solubility of CO_2 are as shown below, the first figure is the targeted output value and secondly is the predicted value generated from the model.

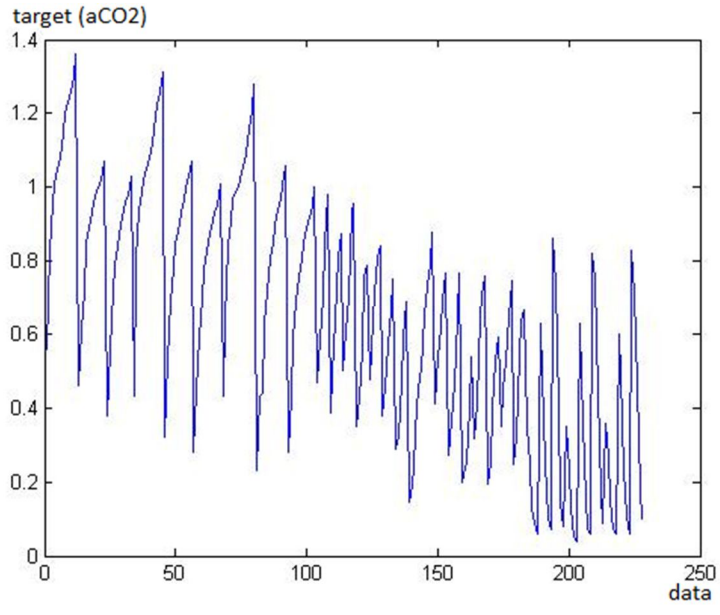


Figure 4.3 : CO_2 loading target

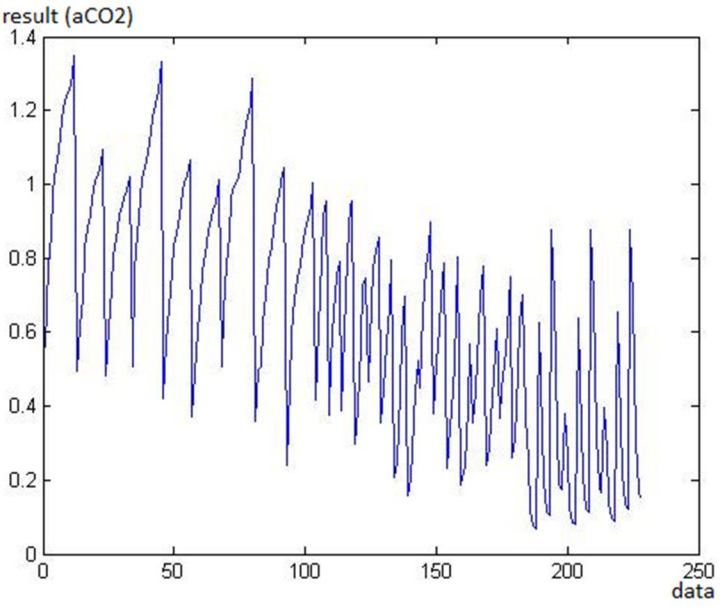


Figure 4.4 : CO_2 loading result

Thus, the comparison of CO_2 loading from prediction and experimental data is obtained. Results from MATLAB shows that the error is ranging from -0.1293 to 0.1544. So, graph below illustrate the deviation of the prediction data.

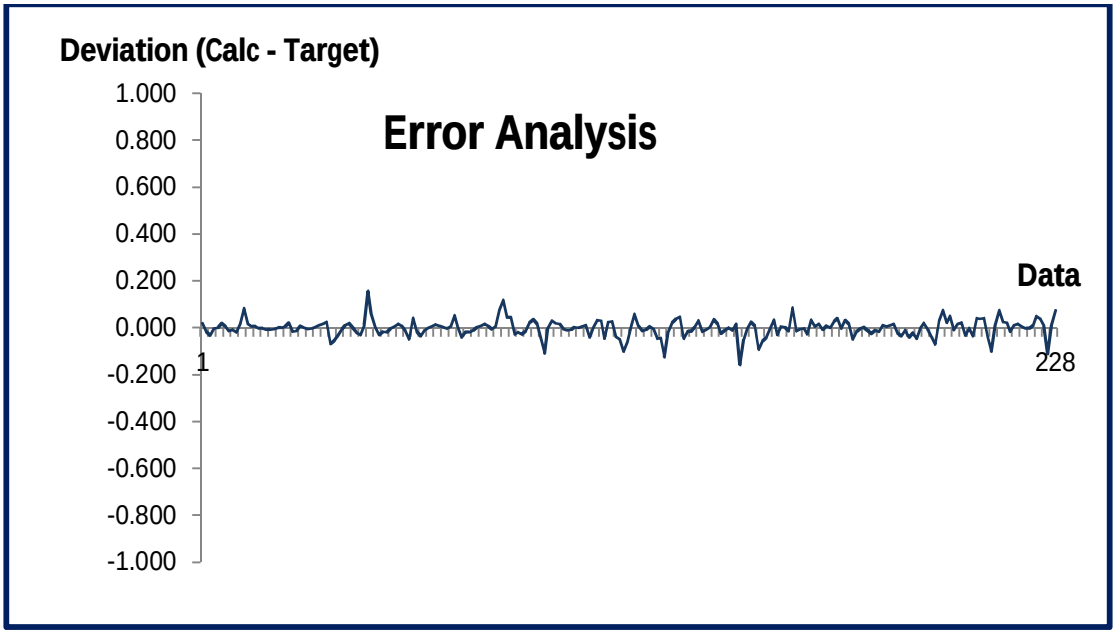


Figure 4.5 : Error analysis of CO_2 loading from experimental data and prediction from neural network model

A small error of deviation is observe and the mean square error = 6.53e-4 and regression = 9.97e-1is obtained, it shows that the model generated is effective to predict the solubility of CO_2 in MDEA+PZ system and helpful in study of vapor-liquid equilibrium behavior related to MDEA-CO_2-H_2O system. AAD reported from the model is 3.047% which show a very good performance.

Table 4.2: Prediction result of MDEA-CO2-H2O system with other papers

Reference	MDEA Conc (kmol/m3)	PZ Conc (kmol/m3)	Temperature (K)	Pressure (kPa)	AAD% prediction
***This work**	1.35-4.77	0.01-1.55	303-363	0.06-3938.40	3.047
M. Vahidi et al	2.52-4.28	0.36-1.36	313-343	30-5000	8.11
B. Lemoine et al	1.98	0	297.7	20-1636	7.84
H. B. Liu et al	1.35-4.77	0.17-1.55	303-363	13.16-935.3	11.6

$$AAD\% = \frac{(Calc\ Value - Exp\ Value)}{Exp\ Value} \times 100\%$$

From the table, the temperature variance is from 303 – 363 (K) which the same range as H. B. Liu et al. which is the widest range and pressure from 0.06 – 3938.40 (kPa), which is the pressure range used during the training process. It can be seen that the prediction results for our own model was more accurate comparing to other model which are 3.047% deviation. The other models reported with higher deviation compare to neural model which we can conclude that neural network model is a great method to predict the solubility of CO_2 in MDEA+PZ system.

Furthermore, other model was developed including data points in absence of Piperazine in the amine aqueous solution, PZ=0. 28 experimental data was added to the system for training process which gives total data for modeling of 256 data. Same method was applied in the model development with neuron number set to 10 for the model simulation. The behavior of the model towards CO_2 loading prediction is as follow.

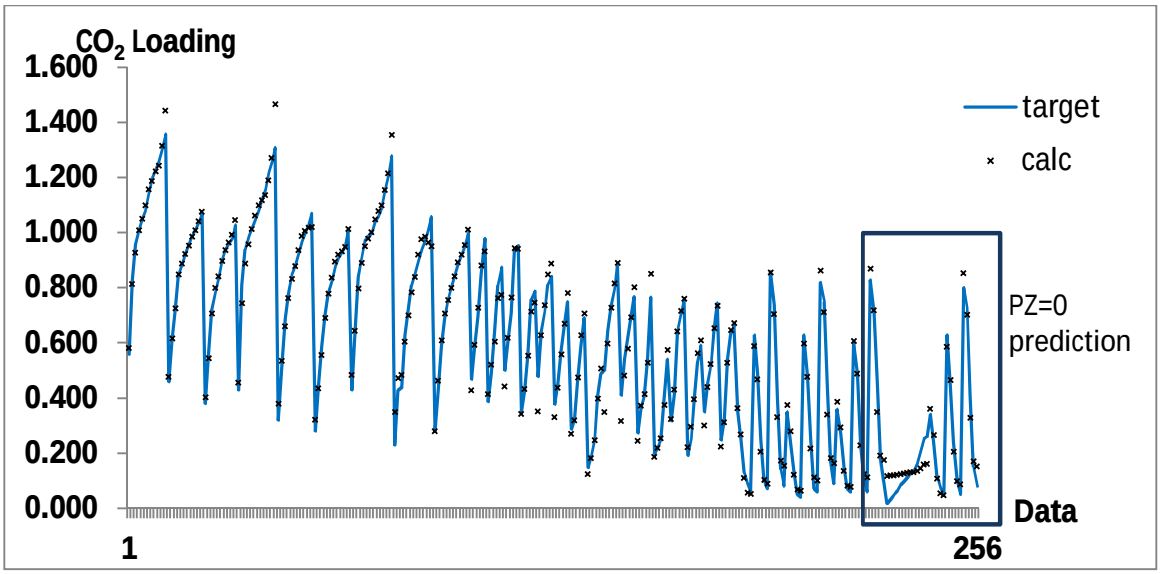


Figure 4.5 : Comparison of CO_2 loading from experimental data and prediction from neural network model

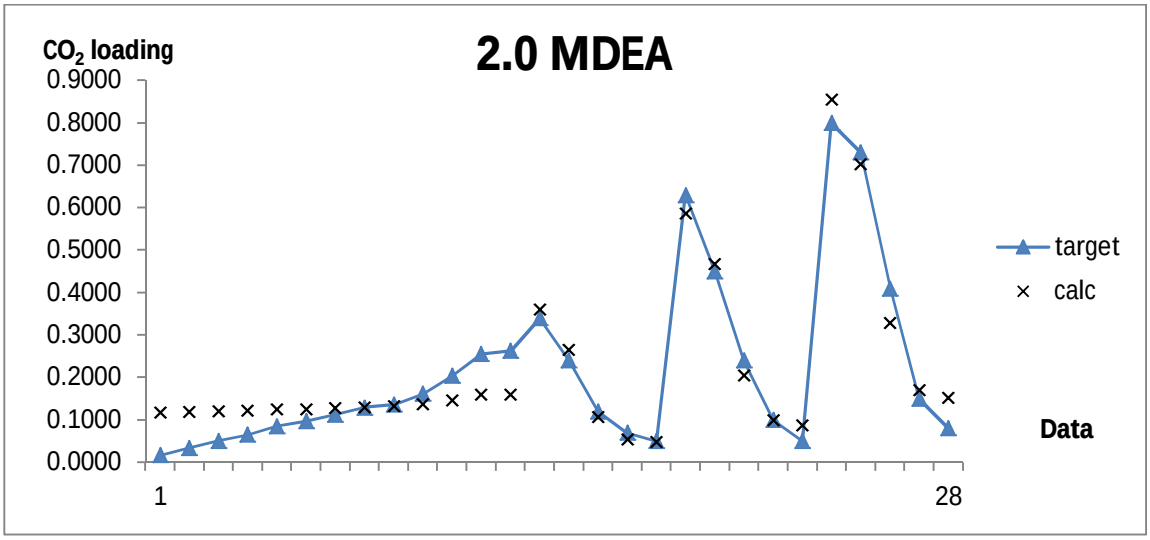


Figure 4.6 : CO_2 loading prediction at PZ=0

The diagram above represents the prediction of CO_2 when PZ is set to zero and the performance reported is 44.72%. There are large discrepancies among the measured data and the experimental solubility data from different authors. The artificial neural network model developed can be used only to correlate the CO_2 solubility of MDEA + PZ system. But the model cannot be used to predict the system in absence of PZ in this case. On other side, the model can accurately predict CO_2 loading in MDEA + PZ system at AAD of 3.047%.

CHAPTER 5

CONCLUSION & RECOMMENDATION

The current processes for CO_2 absorption are used on a large scale. Most processes are based on well-known data and mostly refer to research paper established by many ways of modeling. In this project, the main focus will be on performance comparison of CO_2 solubility in MDEA+PZ aqueous solutions and MDEA aqueous solutions by a well-known model approach; which is artificial neural network model to predict the solubility of CO2 in MDEA-CO_2-H_2O system.

In this study, the new correlation data of the solubility of CO_2 were obtained from the neural network model developed of MDEA-PZ-CO_2-H_2O system at AAD of 3.047%. Concentration of MDEA in this work are from (1.35-4.77) kmol/m^3 and concentration of PZ from (0.01-1.55) kmol/m^3 when the temperature are (303-363) K and partial pressure of CO_2 from (0.06-3938.40) kPa, respectively. Comparing the range of CO2 loading with the study done by Vahidi, Lemoine and Liu this study shown a wider range of prediction data and better model prediction. However, this model is not capable to predict in a zero promoter system.

There are two recommendations that can be applied to improve this mathematical system. The first method is by adding more experimental data to the system so that the neural model can learn the patterns of the output more accurate and precise and make sure that the models were trained at every operating parameter as the extrapolation prediction will be more accurate. Secondly, to predict on zero promoter system, a different new model need to be developed and the data range should only consist of experimental data without the promoter.

REFERENCES

MSU Science Theatre. (1994, August 31). Retrieved October 20, 2012, from http://www.pa.msu.edu/sciencet/ask_st/083194.html

B. Lemoine, Y.-G. L. (2000). Fluid Phase Equilibria 172. *Partial vapor pressure of CO2 and H2S over aqueous methyldiethanol solutions*, 261-277.

B. Si. Ali, M. K. (2004). Effect of Piperazine on CO2 Loading in Aqueous Solutions of MDEA at Low Pressure. *Int. Journal of Thermophysics, Vol 25*, No. 6.

Chih-Yuan Lin, A. N.-H. (2009). Jour. of the Tai. Ins. of Chem. Eng. 40. *Kinetics study of carbon dioxide absorption into aqueous solutions containing N-methyldiethanol + diethanolamine*, 403-412.

Citizendium. (n.d.). Retrieved June 25, 2012, from http://en.citizendium.org/wiki/Acid_gas

Deshmukh, R. D., & Mather, A. E. (1981). A Mathematical model for Equilibrium Solubility of Hydrogen Sulphide and Carbon Dioxide in Aqueous Alkanolamine Solutions. *Chem. Eng. Sci. 36*, 355.

Hua-Bing Liu, C.-F. Z.-W. (1999). A Study on Equilibrium Solubility for Carbon Dioxide in Methyldiethanolamine-Piperazine-Water Solution. *Ind. Eng. Chem. Res. 38*, 4032-4036.

Jiun-Jie Ko, M.-H. L. (2000). Chemical Engineering Science 55. *Kinetics of absorption of carbon dioxide into solutions of N-methyldiethanolamine + water*, 4139-4147.

Kai, Q. Z. (2009). Chinese Journal of Chem. Eng. 17(4). *Modeling and Kinetic Study on Absorption of CO2 by Aqueous Solutions of N-methyldiethanol in a Modified Wetted Wall Column*, 571-579.

Lensen, R. (2004). The promoter effect of piperazine on the removal of carbon dioxide. 10-15.

M. Appl, H. J. (1980). Canadian Patent 1090 098. *Removal of CO2 and/or H2S and/or COS from gases containing these constituents*.

M. Z. Haji-Sulaiman, M. K. (1996). Gas. Sep. Purif. Vol. 10. No. 1. *Equilibrium concentration profiles of species in CO2-alkanolamine-water systems*, 13-18.

Manuel A. Pacheco, S. K. (2000). Chem. Eng. Science 55 . *CO2 absorption into aqueous mixtures of diglycolamine and methldiethanol*, 5125-5140.

Mehdi Vahidi, N. S. (2009). J. Chem. Thermodynamics 41. 1272-1278.

Nielsen, F. (2001). Neural Networks - algorithms and applications. 1-21.

Shakhashiri, P. (2008). Chemical of the week. *Carbon Dioxide, CO2*.

Versteeg, G. F. (1988a). Journal of Chem. Eng. Data 33 (1). *Solubility and diffusivity of acid gas (CO2, NO2) in aqueous alkanolamine solutions*, 29-34.

APPENDICES

Appendix 1

BOC GASES

MATERIAL SAFETY DATA SHEET

PRODUCT NAME: CARBON DIOXIDE, GAS

1. Chemical Product and Company Identification

BOC Gases,
Division of
The BOC Group, Inc.
575 Mountain Avenue
Murray Hill, NJ 07974

TELEPHONE NUMBER: (908) 464-8100
24-HOUR EMERGENCY TELEPHONE NUMBER:
CHEMTREC (800) 424-9300

BOC Gases
Division of
BOC Canada Limited
5975 Falbourne Street, Unit 2
Mississauga, Ontario L5R 3W6

TELEPHONE NUMBER: (905) 501-1700
24-HOUR EMERGENCY TELEPHONE NUMBER:
(905) 501-0802
EMERGENCY RESPONSE PLAN NO: 20101

PRODUCT NAME: CARBON DIOXIDE, GAS
CHEMICAL NAME: Carbon Dioxide
COMMON NAMES/SYNONYMS: Carbonic Anhydride
TDG (Canada) CLASSIFICATION: 2.2
WHMIS CLASSIFICATION: A

PREPARED BY: Loss Control (908)464-8100/(905)501-1700
PREPARATION DATE: 6/1/95
REVIEW DATES: 6/7/96

2. Composition, Information on Ingredients

INGREDIENT	% VOLUME	PEL-OSHA[1]	TLV-ACGIH[2]	LD_{50} or LC_{50} Route/Species
Carbon Dioxide FORMULA: CO_2 CAS: 124-38-9 RTECS #: FF6400000	99.8 TO 99.999	5000 ppm TWA	5000 ppm TWA 30,000 ppm STEL	Not Available

[1] As stated in 29 CFR 1910, Subpart Z (revised July 1, 1993)
[2] As stated in the ACGIH 1994-95 Threshold Limit Values for Chemical Substances and Physical Agents

3. Hazards Identification

EMERGENCY OVERVIEW

Oxygen levels below 19.5% may cause asphyxia. Carbon dioxide exposure can cause nausea and respiratory problems. High concentrations may cause vasodilation leading to circulatory collapse.

PRODUCT NAME: CARBON DIOXIDE, GAS

ROUTE OF ENTRY:

Skin Contact	Skin Absorption	Eye Contact	Inhalation	Ingestion
Yes	No	Yes	Yes	Yes

HEALTH EFFECTS:

Exposure Limits	Irritant	Sensitization
Yes	No	No
Teratogen	**Reproductive Hazard**	**Mutagen**
No	No	No
Synergistic Effects None reported		

Carcinogenicity: – NTP: No IARC: No OSHA: No

EYE EFFECTS:
No adverse effects anticipated.

SKIN EFFECTS:
No adverse effects anticipated.

INGESTION EFFECTS:
No adverse effects anticipated.

INHALATION EFFECTS:
Carbon dioxide is the most powerful cerebral vasodilator known. Inhaling large concentrations causes rapid circulatory insufficiency leading to coma and death. Asphyxiation is likely to occur before the effects of carbon dioxide overexposure. Chronic, harmful effects are not known from repeated inhalation of low concentrations. Low concentrations of carbon dioxide cause increased respiration and headache.

Effects of oxygen deficiency resulting from simple asphyxiants may include: rapid breathing, diminished mental alertness, impaired muscular coordination, faulty judgement, depression of all sensations, emotional instability, and fatigue. As asphyxiation progresses, nausea, vomiting, prostration, and loss of consciousness may result, eventually leading to convulsions, coma, and death.

Oxygen deficiency during pregnancy has produced developmental abnormalities in humans and experimental animals.

NFPA HAZARD CODES

Health: 1
Flammability: 0
Reactivity: 0

HMIS HAZARD CODES

Health: 1
Flammability: 0
Reactivity: 0

RATINGS SYSTEM

0 = No Hazard
1 = Slight Hazard
2 = Moderate Hazard
3 = Serious Hazard
4 = Severe Hazard

4. First Aid Measures

EYES:
Never introduce oil or ointment into the eyes without medical advice! If pain is present, refer the victim to an ophthalmologist for further treatment and follow up.

SKIN:
No adverse effects anticipated.

INGESTION:
Not anticipated.

INHALATION:
PROMPT MEDICAL ATTENTION IS MANDATORY IN ALL CASES OF OVEREXPOSURE TO CARBON DIOXIDE. RESCUE PERSONNEL SHOULD BE EQUIPPED WITH SELF-CONTAINED BREATHING APPARATUS. Conscious persons should be assisted to an uncontaminated area and inhale fresh air. Quick removal from the contaminated area is most important. Unconscious persons should be moved to an uncontaminated area, given mouth-to-mouth resuscitation and supplemental oxygen. Further treatment should be symptomatic and supportive.

5. Fire Fighting Measures

Conditions of Flammability: Nonflammable		
Flash point: None	Method: Not Applicable	Autoignition Temperature: None
LEL(%): None	UEL(%): None	
Hazardous combustion products: None		
Sensitivity to mechanical shock: None		
Sensitivity to static discharge: None		

FIRE AND EXPLOSION HAZARDS:
None. Nonflammable

6. Accidental Release Measures

Evacuate all personnel from affected area. Use appropriate protective equipment. If leak is in user's equipment, be certain to purge piping with inert gas prior to attempting repairs. If leak is in container or container valve, contact the appropriate emergency telephone number listed in Section 1 or call your closest BOC location.

7. Handling and Storage

Electrical Classification:
Non-Hazardous

Dry carbon dioxide can be handled in most common structural materials. Moist carbon dioxide is generally corrosive by its formation of carbonic acid. For applications with moist Carbon Dioxide, 316, 309 and 310 stainless steels may be used as well as Hastelloy ® A, B, & C, and Monel ®. Ferrous Nickel alloys are slightly susceptible to corrosion. At normal temperatures carbon dioxide is compatible with most plastics and elastomers.

Use only in well-ventilated areas. Carbon dioxide vapor is heavier than air and will accumulate in low areas. Valve protection caps must remain in place unless container is secured with valve outlet piped to use point. Do not drag, slide or roll cylinders. Use a suitable hand truck for cylinder movement. Use a pressure reducing regulator when connecting cylinder to lower pressure (<3000 psig) piping or systems. Do not heat cylinder by any means to increase the discharge rate of product from the cylinder. Use a check valve or trap in the discharge line to prevent hazardous back flow into the system.

Protect cylinders from physical damage. Store in cool, dry, well-ventilated area away from heavily trafficked areas and emergency exits. Do not allow the temperature where cylinders are stored to exceed 125°F (52°C). Cylinders should be stored upright and firmly secured to prevent falling or being knocked over. Full and empty cylinders should be segregated. Use a "first in-first out" inventory system to prevent full cylinders being stored for excessive periods of time.

For additional storage recommendations, consult Compressed Gas Association's Pamphlet P-1.

Never carry a compressed gas cylinder or a container of a gas in cryogenic liquid form in an enclosed space such as a car trunk, van or station wagon. A leak can result in a fire, explosion, asphyxiation or a toxic exposure.

Maximum use for potable water 100 mg/l.

8. Exposure Controls, Personal Protection

EXPOSURE LIMITS[1]:

INGREDIENT	% VOLUME	PEL-OSHA[2]	TLV-ACGIH[3]	LD_{50} or LC_{50} Route/Species
Carbon Dioxide FORMULA: CO_2 CAS: 124-38-9 RTECS #: FF6400000	99.8 TO 99.999	5000 ppm TWA	5000 ppm TWA 30,000 ppm STEL	Not Available

[1] Refer to individual state of provincial regulations, as applicable, for limits which may be more stringent than those listed here.
[2] As stated in 29 CFR 1910, Subpart Z (revised July 1, 1993)
[3] As stated in the ACGIH 1994-1995 Threshold Limit Values for Chemical Substances and Physical Agents.

IDLH (Carbon Dioxide): 50,000 ppm

ENGINEERING CONTROLS:
Use local exhaust to prevent accumulation of high concentrations so as to reduce the oxygen level in the air to less than 19.5% and the carbon dioxide concentration below the exposure limit.

EYE/FACE PROTECTION:
Safety goggles or glasses as appropriate for the job.

SKIN PROTECTION:
Protective gloves of any material appropriate for the job.

RESPIRATORY PROTECTION:

Positive pressure air line with full-face mask and escape bottle or self-contained breathing apparatus should be available for emergency use.

OTHER/GENERAL PROTECTION:
Safety shoes.

9. Physical and Chemical Properties

PARAMETER	VALUE	UNITS
Physical state (gas, liquid, solid)	: Gas	
Vapor pressure at 70 °F	: 856	psia
Vapor density at 70 °F, 1 atm (Air = 1)	: 1.53	
Evaporation point	: Not Available	
Boiling point (CO_2 Sublimes)	: -109.3	°F
	: -78.5	°C
Freezing point	: -69.8	°F
	: -56.6	°C
pH	: Not Available	
Specific gravity	: Not Available	
Oil/water partition coefficient	: Not Available	
Solubility (H20)	: Very soluble	
Odor threshold	: Not Applicable	
Odor and appearance	: A colorless, odorless gas.	

10. Stability and Reactivity

STABILITY:
Stable

INCOMPATIBLE MATERIALS:
Certain reactive metals, hydrides, moist cesium monoxide, or lithium acetylene carbide diammino may ignite. Passing carbon dioxide over a mixture of sodium peroxide and aluminum or magnesium may explode.

HAZARDOUS DECOMPOSITION PRODUCTS:
Carbon monoxide and oxygen when heated above 3092 °F (1700°C). Carbonic acid is formed in the presence of moisture.

HAZARDOUS POLYMERIZATION:
Will not occur.

11. Toxicological Information

REPRODUCTIVE:
Oxygen deficiency during pregnancy has produced developmental abnormalities in humans and experimental animals.

Exposure of female rats to 60,000 ppm carbon dioxide for 24 hours has produced toxic effects to the embryo and fetus in pregnant rats. Toxic effects to the reproductive system have been observed in other mammalian species at similar concentrations.

OTHER:

Carbon dioxide is the most powerful cerebral vasodilator known. Inhaling large concentrations causes rapid circulatory insufficiency leading to coma and death. Chronic, harmful effects are not known from repeated inhalation of low (3 to 5 molar %) concentrations.

12. Ecological Information

No data given.

13. Disposal Considerations

Do not attempt to dispose of residual waste or unused quantities. Return in the shipping container PROPERLY LABELED, WITH ANY VALVE OUTLET PLUGS OR CAPS SECURED AND VALVE PROTECTION CAP IN PLACE to BOC Gases or authorized distributor for proper disposal.

14. Transport Information

PARAMETER	United States DOT	Canada TDG
PROPER SHIPPING NAME:	Carbon Dioxide	Carbon Dioxide
HAZARD CLASS:	2.2	2.2
IDENTIFICATION NUMBER:	UN 1013	UN 1013
SHIPPING LABEL:	NONFLAMMABLE GAS	NONFLAMMABLE GAS

15. Regulatory Information

SARA TITLE III NOTIFICATIONS AND INFORMATION

SARA TITLE III HAZARD CLASSES:
Acute Health Hazard
Sudden Release of Pressure Hazard

16. Other Information

Compressed gas cylinders shall not be refilled without the express written permission of the owner. Shipment of a compressed gas cylinder which has not been filled by the owner or with his/her (written) consent is a violation of transportation regulations.

DISCLAIMER OF EXPRESSED AND IMPLIED WARRANTIES:
Although reasonable care has been taken in the preparation of this document, we extend no warranties and make no representations as to the accuracy or completeness of the information contained herein, and assume no responsibility regarding the suitability of this information for the user's intended purposes or for the consequences of its use. Each individual should make a determination as to the suitability of the information for their particular purpose(s).

Appendix 2

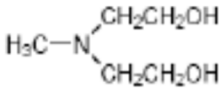
HUNTSMAN

Enriching lives through innovation

Technical Bulletin

METHYLDIETHANOLAMINE (MDEA)

Methyldiethanolamine (MDEA) a clear, water-white, hygroscopic liquid with an ammoniacal odor.



APPLICATIONS

The alkanolamines and their aqueous solutions will absorb carbon dioxide and hydrogen sulfide at lower temperatures and release the acid gases at higher temperatures. This forms the basis for processes which separate carbon dioxide and hydrogen sulfide from gas streams.

Methyldiethanolamine is an alkanolamine used in tail gas treating and hydrogen sulfide enrichment units for selectively removing hydrogen sulfide from gas streams containing carbon dioxide. These units will, in most cases, permit 60 to 80% of the carbon dioxide to remain in the treated gas stream. Methyldiethanolamine is also used in natural gas plants for the bulk removal of carbon dioxide while producing a gas stream containing 0.25 grains hydrogen sulfide/100 scf. Bulk carbon dioxide removal can be realized with methyldiethanolamine when the CO_2:H_2S ratio ranges from 100 to 1,000.

Other suggested uses are urethane catalyst, textile softeners, pH control, and epoxy resin curing agents.

SALES SPECIFICATIONS

Property	Specifications	Test Method*
Appearance	Clear and substantially free of foreign matter	ST-30.1
Color, Pt-Co	150 max.	ST-30.12
Methyldiethanolamine, wt%	99 min.	ST-5.5
Water, wt%	0.5 max.	ST-31.53, 6

*Methods of Test are available from Huntsman Corporation upon request.

ADDITIONAL INFORMATION

Regulatory Information		Typical Physical Properties	
DOT/TDG Classification	Not regulated	Boiling Range, °C	247 (477)
HMIS Code	1-1-0	Flash point, PMCC, °C (°F)	116 (240)
WHMIS Classification	D2B	Freezing Point, °C (°F)	-21 (-5.8)
CAS Number	105-59-9	Specific gravity, 20/20°C	1.0431
		Vapor pressure, 20°C, mm Hg	<0.01
Chemical Control Laws		Viscosity, cSt, 100°F	36.8
US, TSCA	Listed	Weight, lb/gal, 20°C	8.69
Canada, DSL	Listed	Water solubility	Complete

HUNTSMAN

Enriching lives through innovation

TOXICITY AND SAFETY

On the basis of acute studies with laboratory animals, methyldiethanolamine is considered slightly toxic by single oral dose and practically nontoxic by single dermal application. The oral LD_{50} value in the rat is 4.78 g/kg and the dermal LD_{50} value in the albino rabbit is 6.24 g/kg.

Methyldiethanolamine is considered moderately irritating to the eyes, but only slightly irritating to the skin. The product is not corrosive under the conditions of the DOT corrosivity test and is not regulated as a hazardous material for transportation purposes.

Because of the low vapor pressure of methyldiethanolamine, exposure to vapors is not expected to present a significant hazard under normal workplace conditions.

When handling methyldiethanolamine, chemical-type goggles must be worn. In addition, exposed employees should exercise reasonable personal cleanliness, including washing exposed skin areas several times daily with soap and water and laundering soiled work clothing at least weekly.

Should accidental contact with the eyes occur, flush them thoroughly with water for at least 15 minutes and get medical attention. Wash exposed skin areas with soap and water.

For further information on the safe handling of methyldiethanolamine, consult the Material Safety Data Sheet.

HANDLING AND STORAGE

The handling and storage of methyldiethanolamine presents no unusual problems. See the section on toxicity and safety for related additional information.

The solvent properties and alkaline nature of methyldiethanolamine should be considered when installing handling and storage facilities. Methyldiethanolamine will react with copper to form complex salts, so the use of copper and alloys containing copper should be avoided. Carbon steel storage tanks, constructed according to a recognized code, are generally satisfactory.

Carbon steel transfer lines, at least 2 inches in diameter and joined by welds or flanges, are suitable. Screw joints are subject to failure unless back-welded because methyldiethanolamine will leach conventional pipe dopes. U.S. Rubber 899 gasket material or its equivalent is satisfactory for use with flange connections.

Centrifugal pumps are preferred with methyldiethanolamine, although carbon steel rotary pumps can be used. Rotary pumps should be equipped with externally lubricated bearings. A Durametallic Type RO-TT mechanical seal is suitable. Garlock 234, 239, or equivalent can be utilized as pump packing.

AVAILABILITY

Methyldiethanolamine is currently available in 55-gallon drums, tank wagons, and tank cars. Samples are available by contacting our sample department at 1-800-662-0924.

Huntsman Corporation
Business Offices
10003 Woodloch Forest Dr.
The Woodlands, TX 77380
(281) 719-6000

Huntsman Advanced Technology Center
Technical Service
8600 Gosling Rd.
The Woodlands, TX 77381
(281) 719-7780

Samples 1-800-662-0924

www.huntsman.com

5025-0310

Experimental Data of M. Vahidi research paper

T (K)	P (kPa)	C1(kmol/m3)	C2(kmol/m3)	A(Target)	A(Predicted)	%Deviation
313.15	30.50	2.00	1.36	0.560	0.542	-3.160
	120.20	2.00	1.36	0.830	0.834	0.538
	285.00	2.00	1.36	0.960	0.946	-1.510
	553.90	2.00	1.36	1.010	1.016	0.554
	783.40	2.00	1.36	1.050	1.045	-0.509
	1153.00	2.00	1.36	1.080	1.081	0.062
	1703.90	2.00	1.36	1.150	1.137	-1.107
	2063.10	2.00	1.36	1.200	1.179	-1.760
	2495.40	2.00	1.36	1.230	1.232	0.197
	2688.40	2.00	1.36	1.260	1.257	-0.274
	3169.00	2.00	1.36	1.300	1.313	0.974
	3673.70	2.00	1.36	1.360	1.357	-0.189
328.15	45.70	2.00	1.36	0.460	0.467	1.498
	115.40	2.00	1.36	0.610	0.618	1.348
	233.30	2.00	1.36	0.720	0.712	-1.106
	535.20	2.00	1.36	0.850	0.836	-1.703
	750.30	2.00	1.36	0.890	0.882	-0.952
	1017.90	2.00	1.36	0.930	0.920	-1.108
	1306.70	2.00	1.36	0.960	0.952	-0.813
	1736.30	2.00	1.36	0.990	0.995	0.478
	2092.00	2.00	1.36	1.010	1.027	1.659
	2548.60	2.00	1.36	1.040	1.064	2.329
	2987.70	2.00	1.36	1.070	1.097	2.518

343.15	51.60	2.00	1.36	0.380	0.452	18.918
	144.70	2.00	1.36	0.560	0.589	5.165
	336.30	2.00	1.36	0.720	0.713	-0.998
	589.40	2.00	1.36	0.790	0.794	0.546
	832.10	2.00	1.36	0.840	0.835	-0.589
	1311.20	2.00	1.36	0.900	0.908	0.863
	1787.00	2.00	1.36	0.940	0.959	2.030
	2149.60	2.00	1.36	0.960	0.982	2.298
	2521.20	2.00	1.36	0.980	1.003	2.346
	2997.00	2.00	1.36	1.030	1.030	0.032
313.15	27.80	2.50	0.86	0.430	0.453	5.259
	135.30	2.50	0.86	0.810	0.789	-2.575
	344.90	2.50	0.86	0.940	0.922	-1.889
	555.20	2.50	0.86	0.990	0.978	-1.197
	788.30	2.50	0.86	1.020	1.012	-0.756
	1059.20	2.50	0.86	1.050	1.043	-0.688
	1433.60	2.50	0.86	1.080	1.083	0.324
	1825.90	2.50	0.86	1.120	1.127	0.592
	2266.50	2.50	0.86	1.160	1.172	1.024
	2810.50	2.50	0.86	1.220	1.216	-0.310
	3258.60	2.50	0.86	1.260	1.241	-1.487
	3938.40	2.50	0.86	1.310	1.266	-3.337
328.25	38.80	2.50	0.86	0.320	0.368	14.993
	106.40	2.50	0.86	0.530	0.545	2.752
	236.00	2.50	0.86	0.690	0.666	-3.415

	427.70	2.50	0.86	0.780	0.772	-1.024
	682.80	2.50	0.86	0.850	0.851	0.121
	911.00	2.50	0.86	0.880	0.890	1.186
	1281.90	2.50	0.86	0.930	0.928	-0.197
	1782.50	2.50	0.86	0.970	0.964	-0.578
	2108.60	2.50	0.86	1.000	0.986	-1.405
	2465.70	2.50	0.86	1.030	1.009	-2.009
	2990.40	2.50	0.86	1.070	1.044	-2.395
343.15	41.20	2.50	0.86	0.280	0.349	24.713
	99.80	2.50	0.86	0.450	0.471	4.659
	214.30	2.50	0.86	0.590	0.578	-2.053
	385.30	2.50	0.86	0.700	0.687	-1.831
	616.20	2.50	0.86	0.780	0.768	-1.535
	870.00	2.50	0.86	0.830	0.810	-2.459
	1276.80	2.50	0.86	0.880	0.862	-2.097
	1640.10	2.50	0.86	0.910	0.907	-0.289
	2014.50	2.50	0.86	0.930	0.935	0.490
	2408.90	2.50	0.86	0.950	0.954	0.422
	3023.20	2.50	0.86	1.010	0.985	-2.464
313.15	34.00	3.00	0.36	0.430	0.435	1.191
	74.00	3.00	0.36	0.640	0.619	-3.302
	203.60	3.00	0.36	0.840	0.798	-4.961
	384.20	3.00	0.36	0.910	0.901	-1.001
	689.00	3.00	0.36	0.970	0.972	0.202
	871.70	3.00	0.36	0.990	0.994	0.393

	1030.30	3.00	0.36	1.000	1.009	0.903
	1404.00	3.00	0.36	1.040	1.039	-0.056
	1810.70	3.00	0.36	1.060	1.069	0.831
	2225.80	3.00	0.36	1.090	1.097	0.676
	2869.10	3.00	0.36	1.160	1.148	-1.065
	3268.30	3.00	0.36	1.210	1.190	-1.623
	3850.90	3.00	0.36	1.280	1.285	0.400
328.15	43.00	3.00	0.36	0.230	0.345	49.787
	95.40	3.00	0.36	0.430	0.484	12.579
	102.90	3.00	0.36	0.440	0.496	12.706
	220.80	3.00	0.36	0.630	0.620	-1.537
	357.40	3.00	0.36	0.720	0.714	-0.787
	601.40	3.00	0.36	0.810	0.816	0.691
	845.50	3.00	0.36	0.850	0.870	2.330
	1238.50	3.00	0.36	0.900	0.912	1.289
	1641.80	3.00	0.36	0.940	0.937	-0.281
	1967.30	3.00	0.36	0.970	0.958	-1.254
	2452.60	3.00	0.36	1.010	0.994	-1.554
	2943.50	3.00	0.36	1.060	1.044	-1.503
343.15	36.00	3.00	0.36	0.280	0.262	-6.386
	157.80	3.00	0.36	0.430	0.455	5.772
	326.70	3.00	0.36	0.590	0.591	0.113
	514.90	3.00	0.36	0.690	0.698	1.199
	735.50	3.00	0.36	0.760	0.765	0.694
	987.20	3.00	0.36	0.810	0.802	-0.979

1245.70	3.00	0.36	0.850	0.832	-2.110
1644.20	3.00	0.36	0.890	0.887	-0.379
2014.50	3.00	0.36	0.920	0.924	0.385
2476.50	3.00	0.36	0.950	0.958	0.861
2922.50	3.00	0.36	1.000	1.000	0.017

Experimental Data of H. B. Liu research paper

T (K)	P (kPa)	C1(kmol/m3)	C2(kmol/m3)	A(Target)	A(Predicted)	%Deviation
323.15	21.18	1.53	0.17	0.468	0.417	-10.980
	44.00	1.53	0.17	0.589	0.597	1.315
	89.44	1.53	0.17	0.696	0.738	6.011
	271.90	1.53	0.17	0.851	0.856	0.587
	669.40	1.53	0.17	0.980	0.955	-2.512
343.15	35.43	1.53	0.17	0.387	0.416	7.561
	71.29	1.53	0.17	0.492	0.536	8.969
	148.80	1.53	0.17	0.641	0.633	-1.239
	418.80	1.53	0.17	0.811	0.806	-0.586
	688.80	1.53	0.17	0.876	0.893	1.972
323.15	17.78	1.35	0.35	0.500	0.393	-21.414
	41.14	1.35	0.35	0.609	0.597	-1.921
	89.43	1.35	0.35	0.707	0.754	6.606
	509.40	1.35	0.35	0.936	0.922	-1.525
	586.90	1.35	0.35	0.955	0.936	-2.010
343.15	17.60	1.35	0.35	0.349	0.316	-9.358
	32.07	1.35	0.35	0.427	0.420	-1.548
	71.26	1.35	0.35	0.558	0.560	0.336
	243.80	1.35	0.35	0.759	0.724	-4.661
	296.30	1.35	0.35	0.790	0.755	-4.427
303.15	16.73	3.15	0.35	0.477	0.453	-5.005
	54.24	3.15	0.35	0.642	0.667	3.847
	97.47	3.15	0.35	0.714	0.721	0.914

	247.50	3.15	0.35	0.812	0.779	-4.055
	407.50	3.15	0.35	0.842	0.867	2.960
323.15	23.95	3.15	0.35	0.377	0.377	0.107
	42.97	3.15	0.35	0.455	0.467	2.570
	90.11	3.15	0.35	0.573	0.557	-2.801
	200.10	3.15	0.35	0.665	0.639	-3.952
	422.60	3.15	0.35	0.750	0.772	2.954
343.15	33.86	3.15	0.35	0.287	0.303	5.573
	48.08	3.15	0.35	0.324	0.341	5.370
	178.00	3.15	0.35	0.470	0.465	-1.137
	368.00	3.15	0.35	0.591	0.602	1.926
	573.00	3.15	0.35	0.691	0.711	2.837
363.15	19.88	3.15	0.35	0.147	0.169	14.674
	37.54	3.15	0.35	0.191	0.215	12.545
	82.54	3.15	0.35	0.247	0.265	7.212
	312.50	3.15	0.35	0.407	0.380	-6.573
	482.50	3.15	0.35	0.490	0.502	2.407
303.15	15.60	2.80	0.70	0.506	0.440	-13.026
	48.43	2.80	0.70	0.647	0.659	1.847
	97.45	2.80	0.70	0.733	0.736	0.431
	202.50	2.80	0.70	0.793	0.777	-2.068
	460.00	2.80	0.70	0.880	0.908	3.151
323.15	18.98	2.80	0.70	0.410	0.374	-8.739
	49.60	2.80	0.70	0.540	0.523	-3.059
	90.17	2.80	0.70	0.617	0.595	-3.512

	195.10	2.80	0.70	0.694	0.670	-3.500
	380.10	2.80	0.70	0.768	0.772	0.551
343.15	19.24	2.80	0.70	0.274	0.276	0.580
	52.64	2.80	0.70	0.366	0.392	7.017
	73.14	2.80	0.70	0.410	0.426	3.879
	177.80	2.80	0.70	0.541	0.515	-4.824
	935.30	2.80	0.70	0.766	0.807	5.414
363.15	17.37	2.80	0.70	0.198	0.174	-12.143
	25.37	2.80	0.70	0.221	0.202	-8.660
	37.19	2.80	0.70	0.254	0.232	-8.553
	157.20	2.80	0.70	0.401	0.330	-17.740
	412.20	2.80	0.70	0.540	0.499	-7.578
323.15	42.15	4.77	0.53	0.318	0.348	9.345
	91.15	4.77	0.53	0.415	0.443	6.710
	326.20	4.77	0.53	0.649	0.612	-5.700
	508.70	4.77	0.53	0.706	0.684	-3.170
	753.70	4.77	0.53	0.760	0.730	-3.989
343.15	35.83	4.77	0.53	0.193	0.201	4.334
	75.61	4.77	0.53	0.252	0.268	6.526
	203.10	4.77	0.53	0.396	0.370	-6.656
	460.60	4.77	0.53	0.529	0.563	6.420
	713.10	4.77	0.53	0.592	0.690	16.496
323.15	14.34	3.75	1.55	0.349	0.346	-0.850
	46.49	3.75	1.55	0.454	0.496	9.290
	91.15	3.75	1.55	0.525	0.574	9.303

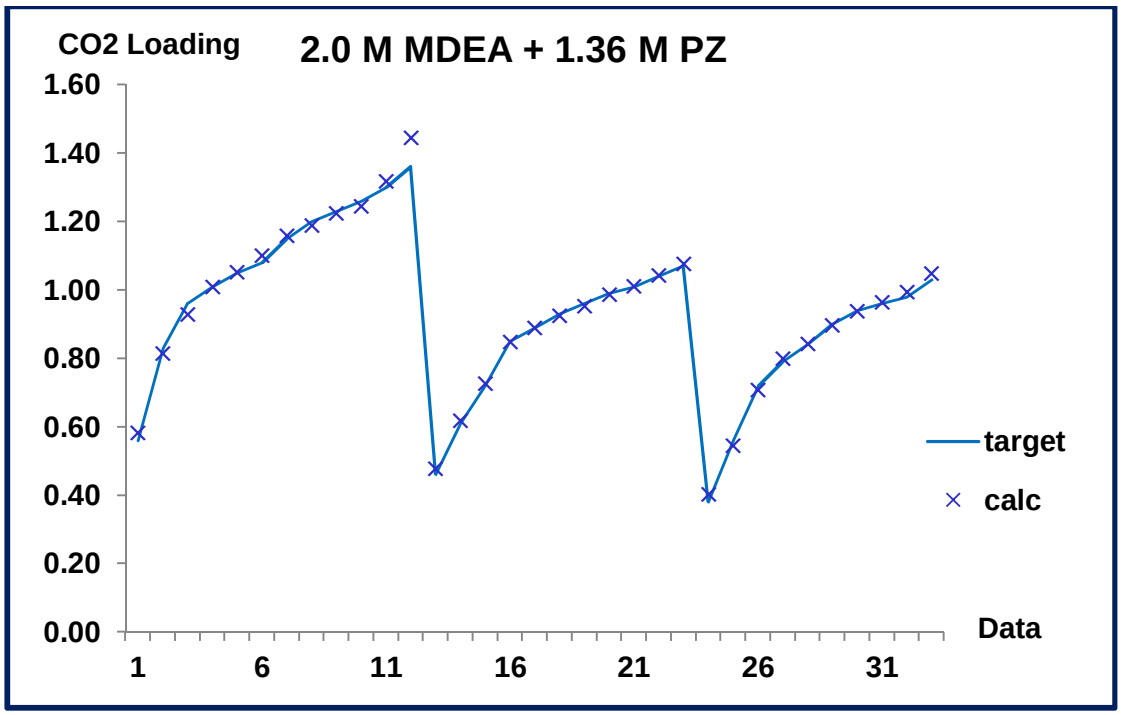
	278.30	3.75	1.55	0.650	0.668	2.745
	678.30	3.75	1.55	0.746	0.736	-1.383
343.15	13.16	3.75	1.55	0.247	0.224	-9.481
	37.35	3.75	1.55	0.323	0.320	-0.956
	224.70	3.75	1.55	0.544	0.526	-3.222
	479.70	3.75	1.55	0.635	0.670	5.563
	667.20	3.75	1.55	0.665	0.723	8.752

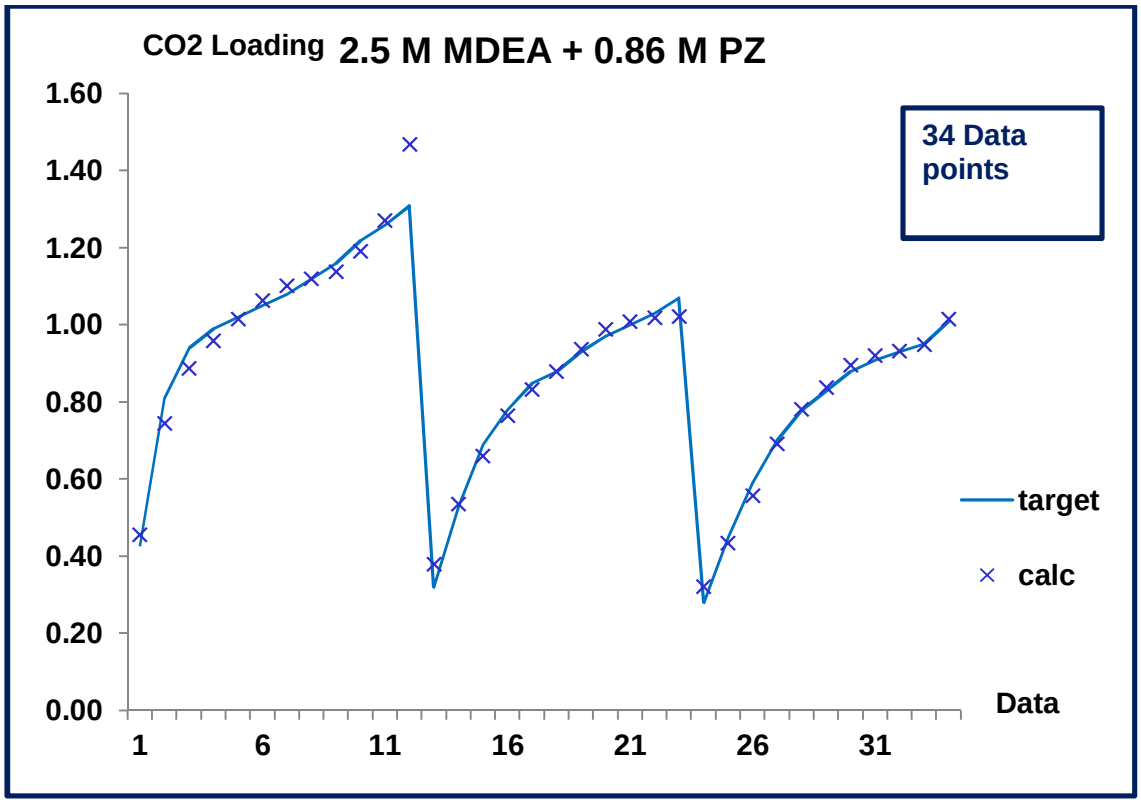
Experimental Data of B. Si Ali research paper

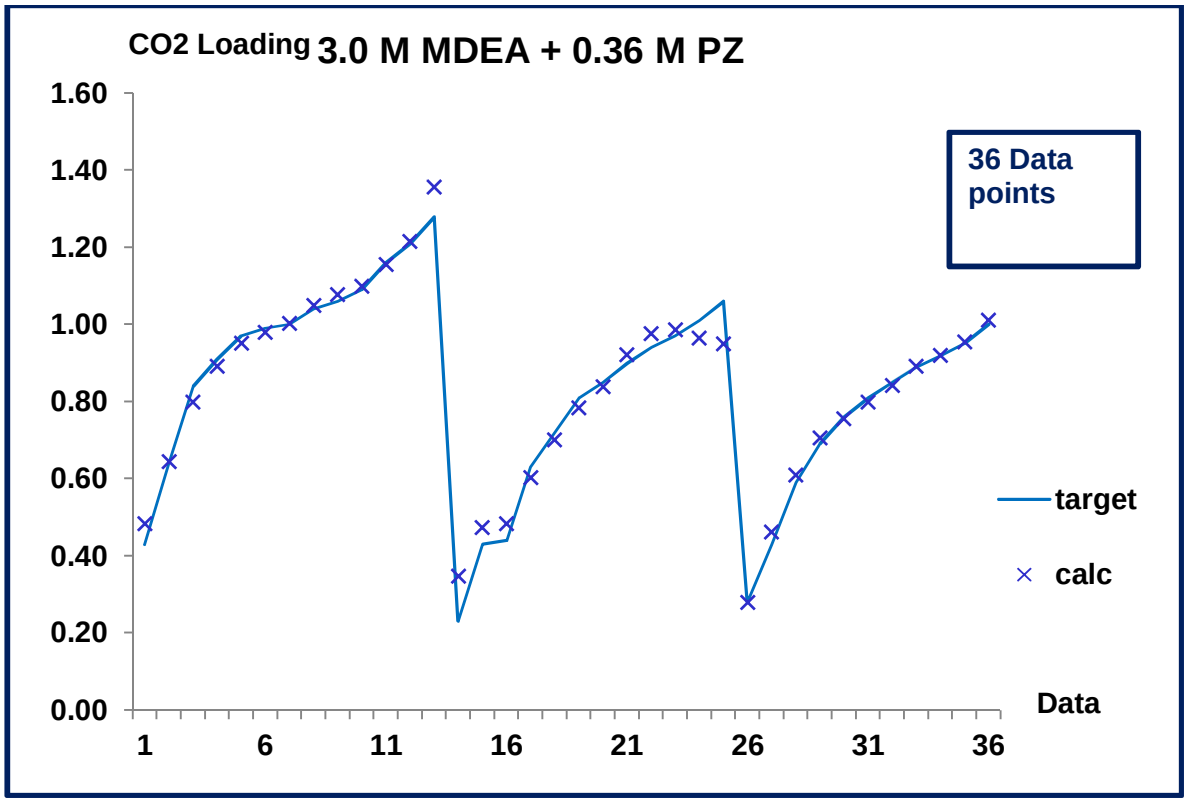
T (K)	P (kPa)	C1(kmol/m3)	C2(kmol/m3)	A(Target)	A(Predicted)	%Deviation
353.15	55.31	1.98	0.01	0.350	0.366	4.655
	27.57	1.98	0.01	0.250	0.271	8.237
	5.55	1.98	0.01	0.130	0.116	-10.818
	0.56	1.98	0.01	0.090	0.064	-28.991
	0.06	1.98	0.01	0.060	0.058	-2.937
333.15	83.07	1.98	0.01	0.630	0.609	-3.363
	41.20	1.98	0.01	0.490	0.484	-1.214
	8.26	1.98	0.01	0.250	0.215	-14.191
	0.83	1.98	0.01	0.100	0.107	7.103
	0.08	1.98	0.01	0.070	0.095	35.494
313.15	95.28	1.98	0.01	0.860	0.860	-0.029
	47.55	1.98	0.01	0.740	0.720	-2.645
	9.54	1.98	0.01	0.400	0.334	-16.505
	0.95	1.98	0.01	0.140	0.164	17.015
	0.10	1.98	0.01	0.080	0.144	80.525
353.15	55.64	1.90	0.05	0.350	0.369	5.508
	27.49	1.90	0.05	0.230	0.271	17.903
	5.55	1.90	0.05	0.130	0.115	-11.541
	0.55	1.90	0.05	0.050	0.062	24.436
	0.06	1.90	0.05	0.040	0.057	41.483
333.15	83.24	1.90	0.05	0.630	0.615	-2.338
	41.28	1.90	0.05	0.480	0.490	2.055
	8.29	1.90	0.05	0.250	0.218	-12.965

	0.83	1.90	0.05	0.070	0.109	55.158
	0.08	1.90	0.05	0.060	0.096	60.365
313.15	95.78	1.90	0.05	0.820	0.868	5.812
	47.55	1.90	0.05	0.750	0.727	-3.047
	9.58	1.90	0.05	0.440	0.338	-23.220
	0.95	1.90	0.05	0.170	0.165	-2.791
	0.10	1.90	0.05	0.090	0.146	61.841
353.15	55.48	1.80	0.10	0.360	0.374	3.780
	27.74	1.80	0.10	0.270	0.276	2.061
	5.58	1.80	0.10	0.150	0.116	-22.703
	0.55	1.80	0.10	0.070	0.062	-11.350
	0.06	1.80	0.10	0.060	0.056	-6.093
333.15	83.07	1.80	0.10	0.600	0.624	3.995
	41.45	1.80	0.10	0.490	0.499	1.787
	8.31	1.80	0.10	0.230	0.222	-3.291
	0.83	1.80	0.10	0.110	0.112	1.552
	0.08	1.80	0.10	0.060	0.099	65.244
313.15	95.78	1.80	0.10	0.830	0.878	5.726
	47.64	1.80	0.10	0.710	0.737	3.782
	9.59	1.80	0.10	0.460	0.343	-25.506
	0.95	1.80	0.10	0.180	0.168	-6.823
	0.10	1.80	0.10	0.100	0.148	47.870

Performance and Analysis of Model






CO2 Loading 3.0 M MDEA + 0.36 M PZ
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
1
6
11
16
21
26
31
36
Data
36 Data points
target
calc

Data Prediction at PZ=0

T (K)	P (kPa)	C1(kmol/m3)	C2(kmol/m3)	A(Target)	A(Predicted)	%Deviation
297.70	20.00	1.98	0.00	0.0171	0.091451	434.803
297.70	62.00	1.98	0.00	0.0342	0.092652	170.911
297.72	114.00	1.98	0.00	0.0512	0.09425	84.083
297.71	165.00	1.98	0.00	0.0648	0.095995	48.141
297.71	256.00	1.98	0.00	0.0853	0.098681	15.687
297.71	304.00	1.98	0.00	0.0971	0.099873	2.856
297.70	402.00	1.98	0.00	0.1126	0.102797	-8.706
297.72	477.00	1.98	0.00	0.1295	0.105265	-18.714
297.73	546.00	1.98	0.00	0.1361	0.107384	-21.099
297.72	716.00	1.98	0.00	0.1617	0.112345	-30.522
297.70	1075.00	1.98	0.00	0.2042	0.122779	-39.873
297.72	1593.00	1.98	0.00	0.2550	0.137587	-46.044
297.67	1636.00	1.98	0.00	0.2625	0.138802	-47.123
353.15	55.48	2.00	0.00	0.3400	0.366374	7.757
353.15	27.57	2.00	0.00	0.2400	0.270576	12.740
353.15	5.56	2.00	0.00	0.1200	0.116491	-2.924
353.15	0.55	2.00	0.00	0.0700	0.064411	-7.984
353.15	0.08	2.00	0.00	0.0500	0.059098	18.196
333.15	82.91	2.00	0.00	0.6300	0.607157	-3.626
333.15	41.37	2.00	0.00	0.4500	0.483687	7.486
333.15	8.31	2.00	0.00	0.2400	0.214653	-10.561
333.15	0.83	2.00	0.00	0.1000	0.106883	6.883

333.15	0.06	2.00	0.00	0.0500	0.094329	88.657
313.15	95.61	2.00	0.00	0.8000	0.858552	7.319
313.15	47.72	2.00	0.00	0.7300	0.719758	-1.403
313.15	9.53	2.00	0.00	0.4100	0.333113	-18.753
313.15	0.96	2.00	0.00	0.1500	0.163779	9.186
313.15	0.10	2.00	0.00	0.0800	0.144202	80.253